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Coarse-grained simulations of material shock compression: interplay between mechanics, thermals, and chemistry

Antillon, Edwin, eantillo@purdue.edu, Purdue University, United States

ABSTRACT

We present a coarse-graining model that enables the description of pressure-induced, endothermic reactions in a model material. An additional implicit variable (the particle size) is used to describe particles undergoing volume-reducing endothermic reactions via a bistable intra-molecular potential, whereas the dynamics of the center-of-mass motion evolves according to interparticle forces. The equations of motion are derived from a Hamiltonian and the model exhibits two desired features: total energy conservation and Galilean invariance. In this study, we explore a simple model material with pairwise interactions between particles to study pressure-induced chemical reactions under both quasi-static and shock loading conditions. Our results demonstrate that such model can capture the complex mechanical processes arising from the interplay between deformation defects and chemical reactions. Moreover, we explore the feasibility to realize a material with such characteristics that can be used to attenuate the energy in sustained shocks which is of interest in many applications.